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Exercise Sheet 6

Aim: *Visualising of protein structures and of protein-ligand interactions, Evaluation of homology models*

Protein structure: Homology modelling

For the interactive material for this exercise follow this link:

https://service.bioinformatik.uni-saarland.de/sww/tutorial-6.php

Exercise 6.1: Homology modelling

The follow the link
1. Punktmutationen in cAPK

(1) From which organism does the sequence originate?
(2) Which organism was used for the expression of the protein?
(3) What is the reported maximum (best) resolution of the X-ray structure?
(4) Which other (non-protein) molecules are present in the structure?
(5) Determine the corresponding UniProt accession number of this protein.

Investigate 1ATP.pdb (using a Visualisation program of your choice or directly on the website via 3D View)
(6) Find the active centre
(7) What is „chain E“ and what is „chain I“ ?
(8) Which consequences would you expect upon the exchange of Asp166 by Ala? Carry out this mutation on the corresponding FASTA sequence using a text editor.
(9) Compare the obtained homology model to that of the wild-type. Please note that the numbering of the residues might have changed if the first amino acid within the X-ray did not start at 1. Are there are crucial changes notable in the structure of the protein?

Remark: For the second project you will need a program to visualize protein structures (.pdb files), such as VMD, PyMol, USCF Chimera, SWISS-PDB Viewer / DeepView,…

To start VMD on the CIP-Pool computers first open a terminal window or console, and enter following comand line (press the enter key):

`vmd` or `/usr/local/bin/vmd`